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June 9, 2008

Physical Review C

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Ab-initio shell model with a core

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(Dated: June 4, 2008)

We construct effective 2- and 3-body Hamiltonians for the p-shell by performing $12\hbar\Omega$ *ab initio* no-core shell model (NCSM) calculations for $A=6$ and 7 nuclei and explicitly projecting the many-body Hamiltonians onto the $0\hbar\Omega$ space. We then separate these effective Hamiltonians into 0-, 1- and 2-body contributions (also 3-body for $A=7$) and analyze the systematic behavior of these different parts as a function of the mass number A and size of the NCSM basis space. The role of effective 3- and higher-body interactions for $A > 6$ is investigated and discussed.

PACS numbers: 21.10.Hw, 23.20.En, 23.20.Lv, 23.20.-g, 27.40.+z

Keywords: NCSM, *ab-initio*, effective interactions

I. INTRODUCTION

Microscopic *ab-initio* many-body approaches have significantly progressed in recent years [1–8]. Nowadays, due to increased computing power and novel techniques, *ab-initio* calculations are able to reproduce a large number of observables for atomic nuclei with mass up to $A=14$. The light nuclei have also served as a crucial site to recognize the important role of three-body forces and three-body correlations. Approaches like the No-Core Shell Model (NCSM) [5], the Green's Function Monte Carlo (GFMC) [6] and the Coupled-cluster theory with single and double excitations (CCSD) [8] can be formally extended for heavier nuclei. However, the explosive growth in computational power, required to achieve convergent results, severely hinders the detailed *ab-initio* studies of heavier, $A \geq 16$, nuclei. In the case of the NCSM, the slow convergence of the calculated energies is caused by the adoption of a two-body cluster approximation, which does not take many-body correlations into account. Straight-forward employment of the three-body and higher-body interactions dramatically complicates the problem, even for light nuclei.

An alternative approach is to construct a small-space effective two-body interaction, which would account for the many-body correlations for the A -body system in a large space. Attempts to include many-body correlations approximately modifying the one-body part of the effective two-body Hamiltonian and employing a unitary transformation have been reported recently [9].

In this paper we derive a valence space ($0\hbar\Omega$) effective two-body interaction that accounts for all the core-polarization effects available in the *ab-initio* NCSM wavefunctions.

First, in the framework of the NCSM, we construct the effective Hamiltonians on the two-body cluster level for

$A=6$ systems in the $N_{\max}\hbar\Omega$ space. N_{\max} represents the limit on the total oscillator quanta (N) above the minimum configuration. We take N_{\max} values from 2 to 12. Second, following the original idea of Ref. [10], we employ an unitary many-body transformation and obtain the effective two-body Hamiltonian in the $0\hbar\Omega$ space (p-space), which exactly reproduces the lowest, $0\hbar\Omega$ space dominated, eigenstates of the 6-body Hamiltonian in the large $N_{\max}\hbar\Omega$ space. Third, we perform NCSM calculations for $A=4$ and $A=5$ systems with the effective Hamiltonian constructed on the two-body cluster level for the $A=6$ system and determine the core and one-body parts of the effective two-body Hamiltonian for $A=6$ in the p-space. Finally, the procedure is generalized for arbitrary mass number A . We analyze the properties of the constructed two-body Hamiltonians, investigate their efficiency to reproduce the observables of different A -body systems calculated in large $N_{\max}\hbar\Omega$ spaces and study the role of the effective p-space three-body interaction.

II. APPROACH

A. No Core Shell Model and effective interaction

The starting point of the No Core Shell Model (NCSM) approach is the bare, exact A -body Hamiltonian constrained by the Harmonic Oscillator (HO) potential [5]:

$$H_A^\Omega = \sum_{j=1}^A h_j^\Omega + \sum_{j>i=1}^A V_{ij}(\Omega, A), \quad (1)$$

where h_j^Ω is the one-body HO Hamiltonian

$$h_j^\Omega = \frac{p_j^2}{2m} + \frac{1}{2}m\Omega^2 r_j^2 \quad (2)$$

and $V_{ij}(\Omega, A)$ is a bare NN interaction V_{ij}^{NN} modified by the term introducing A - and Ω -dependent corrections to

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offset the HO potential present in h_j^Ω :

$$V_{ij}(\Omega, A) = V_{ij}^{NN} - \frac{m\Omega^2}{2A}(\vec{r}_i - \vec{r}_j)^2. \quad (3)$$

The eigenvalue problem for the exact A-body Hamiltonian (1) for $A > 3$ is very complicated technically, since an extremely large A-body HO basis is required to obtain converged results. However, the $A = 2$ problem is considerably simpler. For many realistic NN interactions its solution in the relative HO basis with $N_{\max} = 450$ accounts well for the short range correlations and is a precise approximation for the infinite space ($N_{\max} \rightarrow \infty$) result. This allows one to adopt the two-body cluster approximation to construct the NCSM effective two-body Hamiltonian $H_{A,a=2}^{N_{\max},\Omega}$ for an A-body system in an $N_{\max}\hbar\Omega$ space of tractable dimension, where the lower index a stands for the number of particles in the cluster. This approximation consists of solving Eq.(1) for the $a = 2$ body subsystem of A leading to

$$H_{A,a=2}^\Omega = h_1^\Omega + h_2^\Omega + V_{12}(\Omega, A). \quad (4)$$

The information about the total number of interacting particles A enters the bare $H_{A,a=2}^\Omega$ Hamiltonian through the second term in the right hand side of (3). Next, we find the unitary transformation U_2 which reduces the bare $H_{A,a=2}^\Omega$ Hamiltonian in the “infinite space” ($N_{\max}^\infty = 450$) to the diagonal form:

$$E_{A,2}^\Omega = U_2 H_{A,2}^\Omega U_2^\dagger, \quad (5)$$

where, for the sake of simplicity, we omit the index A for U_2 and keep only the index a indicating the order of cluster approximation. The matrix U_2 can be split into 4 blocks:

$$U_2 = \begin{pmatrix} U_{2,P} & U_{2,PQ} \\ U_{2,QP} & U_{2,Q} \end{pmatrix}, \quad (6)$$

where the square $d_P \times d_P$ $U_{2,P}$ matrix corresponds to the P-space (or model space) of dimension d_P , characterized by the chosen N_{\max} value.

Taking into account that the $E_{A,2}^\Omega$ matrix has a diagonal form

$$E_{A,2}^\Omega = \begin{pmatrix} E_{A,2,P}^\Omega & 0 \\ 0 & E_{A,2,Q}^\Omega \end{pmatrix}, \quad (7)$$

one can calculate the effective $H_{A,2}^{N_{\max},\Omega}$ Hamiltonian using the following formula:

$$H_{A,2}^{N_{\max},\Omega} = \frac{U_{2,P}^\dagger}{\sqrt{U_{2,P}^\dagger U_{2,P}}} E_{A,2,P}^\Omega \frac{U_{2,P}}{\sqrt{U_{2,P}^\dagger U_{2,P}}}. \quad (8)$$

It is easy to show by inserting Eq.(5) into the Eq.(8), and taking into account Eq.(6) that the unitary transformation (8) is equivalent to the commonly used unitary

transformation [11, 12] and that Eq.(8) is identical to the Eqs.(15,16) from [5]. We note, that, by using Eq.(8) one does not need to calculate and store a large number of matrix elements of the ω -operator (i.e., $U_{2,P}^\dagger \omega_2 = U_{2,PQ}^\dagger$). Furthermore, the decoupling condition $QH^{\text{eff}}P = 0$ is automatically satisfied, which is obvious from the diagonal form of the $E_{A,2}^\Omega$ matrix. We note that our treatment of center-of-mass motion remains the same as in the NCSM (Ref. [5]). We initiate all effective interaction developments at the A-body level, and, through a series of steps, arrive at a smaller space effective interaction appropriate for the A-body system. For this reason, our derived effective Hamiltonians have their first subscript as “A”.

B. Projection of the many-body Hamiltonian

The next step of the traditional NCSM prescription is to construct the full A-body Hamiltonian using the effective two-body Hamiltonian (8) and to diagonalize it in the A-body N_{\max} model space. As we increase the number of nucleons, the dimension of the corresponding N_{\max} model space increases very rapidly. For instance, up-to-date computing resources allow us to go as high as $N_{\max} = 16$ for the lower part of the p-shell ($A=5,6$) [13], while already for the upper part of the p-shell ($A \sim 15$), we are limited to $N_{\max} = 8$. The computational eigenvalue problem for many-body systems is complicated because of the very large matrix dimensions involved. The largest dimension of the model space that we encountered in this study for ${}^6\text{Li}$ with $N_{\max} = 12$ exceeds $d_P = 4.8 \times 10^7$. To solve this problem we have used the specialized version of the shell-model code ANTOINE [14, 15], recently adapted for the NCSM [16].

In fact, the NCSM calculation for the $A=6$ system in the $N_{\max} = 12$ space yields nearly converged energies for the lowest states dominated by the $N = 0$ components, while there is incomplete convergence for $A \geq 15$ in $N_{\max} = 8$ space. Therefore, considering the $N_{\max} = 12$ NCSM results as exact solutions for the lowest $N = 0$ dominated 6-body states, we may construct the $N_{\max} = 0$ space Hamiltonian for the $A=6$ system, which exactly reproduces those $N_{\max} = 12$ eigenvalues [10]. Moreover, if it is possible to solve the 6-body problem for $A=6$, then it is possible to solve the 6-body problem for arbitrary A, using the corresponding effective Hamiltonian $H_{A,2}^{N_{\max},\Omega}$ obtained in the two-body cluster approximation. This means that we can determine for any A-body system the effective Hamiltonian in the $N_{\max} = 0$ space, which accounts for 6-body cluster dynamics in the large $N_{\max} = 12$ space.

To generalize, we start by defining the procedure for determining the effective Hamiltonian matrix elements for the a_1 -body cluster in the A-nucleon system. We do this by constructing the full a_1 -body Hamiltonian using the effective 2-body Hamiltonian (8) and diagonalizing it in the N_{\max} model space. In the spirit of Eq.(5), this

yields the eigenenergies $E_{A,a_1}^{N_{\max},\Omega}$ of the a_1 -body system and their corresponding a_1 eigenvectors which make up the unitary transformation matrix $U_{a_1,P}^{A,N_{\max}}$. These a_1 -body results can then be projected into a smaller, secondary P_1 -space, given by $N_{1,\max}\hbar\Omega$ with $N_{1,\max} = 0$, where, similar to Eqs.(6) and (7), $E_{A,a_1}^{N_{\max},\Omega}$ and $U_{a_1,P}^{A,N_{\max}}$ can be split into parts related to the two spaces, P_1 and Q_1 , where $P_1 + Q_1 = P$. The new secondary effective Hamiltonian then takes the following general form:

$$\mathcal{H}_{A,a_1}^{N_{1,\max},N_{\max}} = \frac{U_{a_1,P_1}^{A,\dagger}}{\sqrt{U_{a_1,P_1}^{A,\dagger} U_{a_1,P_1}^A}} E_{A,a_1}^{N_{\max},\Omega} \frac{U_{a_1,P_1}^A}{\sqrt{U_{a_1,P_1}^{A,\dagger} U_{a_1,P_1}^A}}, \quad (9)$$

where the Ω superscript on the left-hand side is omitted for the sake of simplicity. As stated earlier, the new index a_1 determines the order of the cluster approximation in the smaller P_1 space, *i.e.*, $N_{1,\max} = 0$. Because the P_1 space has $N_{1,\max} = 0$, the projection into this space "freezes" some number of the a_1 nucleons into fixed single particle configurations, which can be thought of as the "inert core" states in the Standard Shell Model (SSM) approach. Consequently, it is possible to write a_1 as $a_1 = A_c + a_v$, where A_c is the number of nucleons making up the core configuration, while a_v refers to the size of valence cluster.

For instance, in the case of p-shell nuclei, $A_c = 4$, so, if $a_1 = 5$ (*i.e.* the 5-body cluster approximation), then the effective Hamiltonian $\mathcal{H}_{A,a_1=5}^{N_{1,\max}=0,N_{\max}}$ is simply a one-body Hamiltonian ($a_v = 1$) appropriate for the A-nucleon system. Similarly, for the 6-body cluster approximation, *i.e.*, $a_1 = 6$, we obtain the effective Hamiltonian $\mathcal{H}_{A,a_1=6}^{N_{1,\max}=0,N_{\max}}$, which is a two-body Hamiltonian ($a_v = 2$) for the A-body system, and, so on for larger values of a_1 . Whatever the value of a_v is, the effective Hamiltonian $\mathcal{H}_{A,a_1}^{N_{1,\max}=0,N_{\max}}$ contains the information about the a_1 -body dynamics in the original large $N_{\max}\hbar\Omega$ space, since it reproduces exactly the lowest d_{P_1} eigenvalues $E_{A,a_1}^{N_{\max},\Omega}$ of the a_1 -body Hamiltonian in the $N_{\max}\hbar\Omega$ space, where d_{P_1} is a dimension of the P_1 space.

In the case of a doubly magic closed shell with two extra nucleons *i.e.*, $A = 6, 18, 42$, *etc.*, the dimension of the effective Hamiltonian $\mathcal{H}_{A,a_1=A}^{0,N_{\max}}$ is a 2-body ($a_v = 2$) Hamiltonian in the p-, sd-, pf-spaces, *etc.*, respectively. This means that the secondary effective Hamiltonian (9) contains only 1-body and 2-body terms, even after the *exact* A-body cluster transformation. This effective Hamiltonian (9), which now contains the correlation energy of all A nucleons, is the correct one-body plus two-body Hamiltonian to use in a SSM calculation with inert core. The $A_c = A - 2$ nucleon-spectators fully occupy the shells below the valence shell and the total A-body wavefunction can be exactly factorized as the A_c -body "core" and the valence 2-body wave functions. This considerably simplifies the calculation of the effective Hamiltonian, because only the $0\hbar\Omega$ part (P_1 -space part) of the complete $N_{\max}\hbar\Omega$ wave function needs to be specified.

III. EFFECTIVE TWO-BODY P-SHELL INTERACTION

Utilizing the approach outlined above, we have calculated effective p-shell Hamiltonians for ${}^6\text{Li}$, using the 6-body Hamiltonians with $N_{\max} = 2, 4, \dots, 12$ and $\Omega = 14$ MeV, constructed from the INOY (inside nonlocal outside Yukawa) interaction [18, 19]. This is a new type of interaction, which has local behavior appropriate for traditional NN interactions at longer ranges, but exhibits a nonlocality at shorter distances. The nonlocality of the NN interaction has been introduced in order to account effectively for three-nucleon (NNN) interactions which correctly describe the NNN bound states ${}^3\text{H}$ and ${}^3\text{He}$, whereas still reproducing NN scattering data with high precision. The corresponding excitation energies of p-shell dominated states and the binding energy of ${}^6\text{Li}$ are shown in Fig.1 as a function of N_{\max} . The dimension of

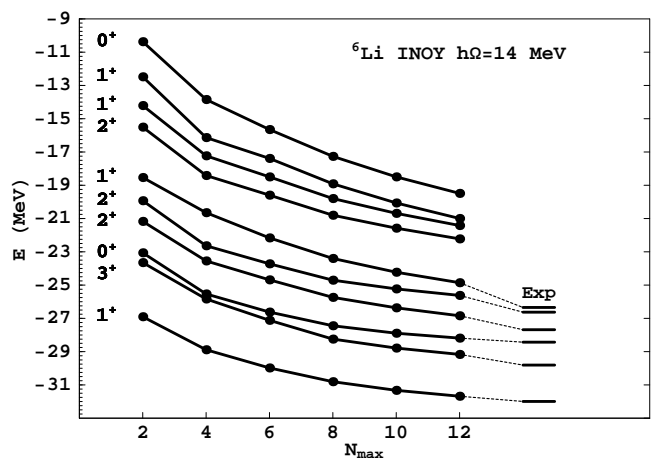


FIG. 1: The excitation energies of the J^π states and ground state energy for ${}^6\text{Li}$ calculated in the $N_{\max}\hbar\Omega$ spaces with the INOY interaction and $\hbar\Omega = 14$ MeV. The experimental spectra and ground state energy are shown for comparison.

the configurational space for the $N_{\max} = 12$ case considered is 48 million (M-scheme). A two orders of magnitude increase in the size of the model space, as compared to the previous $N_{\max} = 6$ study [10], allows us to determine a converged value of 31.681 MeV for the ${}^6\text{Li}$ binding energy. Furthermore, the excitation energy of the highest lying p-space state, $J^\pi = 0_2^+$, is lowered by an amount of 2.1 MeV in comparison to the $N_{\max} = 6$ case, indicating improved convergence for both the excited states and ground state for $N_{\max} = 12$.

In the SSM an effective two-body Hamiltonian for a nucleus with mass number A is represented in terms of three components:

$$H_{\text{SSM}}^A = H_0 + H_1 + V_2^A, \quad (10)$$

where H_0 is the inert core part associated with the interaction of the nucleons occupying closed shells, H_1 is the one-body part corresponding to the interaction of valence

nucleons with core nucleons, and V_2^A is the two-body part referring to the interaction between valence particles. It is usually assumed that the core and one-body parts are constant for an arbitrary number of valence particles and that only the two-body part V_2^A may contain mass dependence that includes effects of three-body and higher-body interactions.

To represent the $\mathcal{H}_{A,a_1}^{0,N_{\max}}$ Hamiltonian in the SSM format, we develop a valence cluster expansion (VCE),

$$\mathcal{H}_{A,a_1}^{0,N_{\max}} = H_0^{A,A_c} + H_1^{A,A_c+1} + \sum_{k=2}^{a_v} V_k^{A,A_c+k}, \quad (11)$$

where the lower index, k , stands for the k -body interaction in the a_v -body valence cluster ($a_1 = A_c + a_v$); the first upper index A for the mass dependence; and the second upper index, $A_c + k$ for the number of particles contributing to the corresponding k -body part. Thus, we consider the more general case of allowing the core ($k=0$), one-body ($k=1$) and other k -body parts to vary with the mass number A . This appears necessary to include the A -dependence of the excitations of the core (A_c) nucleons treated in the original N_{\max} basis space. For the $A=6$ case the two-body valence cluster (2BVC) approximation is exact:

$$\mathcal{H}_{A=6,a_1=6}^{0,N_{\max}} = H_0^{6,4} + H_1^{6,5} + V_2^{6,6}, \quad (12)$$

where the core part, $H_0^{6,4}$, is defined as the ground state $J^\pi = 0^+$ energy of ${}^4\text{He}$ calculated in the $N_{\max}\hbar\Omega$ space with the TBMEs of the primary effective Hamiltonian, $H_{6,2}^{N_{\max},\Omega}$ for $A=6$. Then the one-body part, $H_1^{6,5}$, is determined as

$$H_1^{6,5} = \mathcal{H}_{6,5}^{0,N_{\max}} - H_0^{6,4}. \quad (13)$$

The TBMEs of the one-body part, $H_1^{6,5}$,

$$\langle ab; JT | H_1^{6,5} | cd; JT \rangle = (\epsilon_a + \epsilon_b) \delta_{a,c} \delta_{b,d} \quad (14)$$

may be represented in terms of single particle energies (SPE), ϵ_a :

$$\epsilon_a^p = E({}^5\text{Li}, j_a) - V_0^{6,4}, \epsilon_a^n = E({}^5\text{He}, j_a) - V_0^{6,4}. \quad (15)$$

where the index a (as well as b, c , and d) denotes the set of single particle HO quantum numbers (n_a, l_a, j_a), upper index stands for proton (p) and neutron (n), and the $E({}^5\text{Li}, J)$, $E({}^5\text{He}, J)$ are NCSM energies of the lowest $J_i^\pi = 3/2_1^-$ and $J_i^\pi = 1/2_1^-$ states calculated in the $N_{\max}\hbar\Omega$ space for the 5-body system using the TBMEs of the $A = 6$ effective Hamiltonian, $H_{A=6,2}^{N_{\max},\Omega}$, which includes Coulomb energy. Finally, the two-body part $V_2^{6,4}$ is obtained by subtracting of two Hamiltonians:

$$V_2^{6,6} = \mathcal{H}_{6,6}^{0,N_{\max}} - \mathcal{H}_{6,5}^{0,N_{\max}}. \quad (16)$$

It is worth noting that since the Coulomb energy is included in the original Hamiltonian, the proton-proton

(pp), neutron-neutron (nn) and proton-neutron (pn) $T = 1$ TBMEs of the two-body part, $V_2^{6,6}$, have different values. The pn TBMEs of the core, one-body and two-body parts of the expanded Hamiltonian for ${}^6\text{Li}$ are listed in the Table I. In Table I we also list the values of $H_{6,2}^{N_{\max}=12,\Omega=14}$, so that one can observe how much these values change when the correlations up to 6-bodies are included, so as to obtain the values of $\mathcal{H}_{6,6}^{0,12}$.

The results presented in Table I indicate that the largest parts of the effective Hamiltonian are attributed to the interaction among core nucleons ($k=0$) and the interaction of valence nucleons with the core nucleons ($k=1$). However, these two largest contributions partially cancel each other. The pure two-body part corresponding to the interaction of valence nucleons is considerably smaller than the individual core and one-body parts. Note that one may re-partition the core and single particle energies by shifting a constant amount from $H_0^{A,5}$ to $H_0^{A,4}$. A shift of ≈ 24 MeV (≈ 32 MeV) for $A=6$ (7) produces core and valence energies where the core matches the ${}^4\text{He}$ as in the NCSM with $A=4$.

To investigate the balance of the pure two-body, $V_2^{6,6}$, core, $H_0^{6,4}$, and one-body, $H_1^{6,5}$, parts of the effective Hamiltonian with the increase of the size of the original many-body space, we have plotted the sum of core and one-body parts, $H_0^{6,4} + H_1^{6,5}$, as a function of N_{\max} in Fig.2. The results in Fig.2 reveal a weak dependence

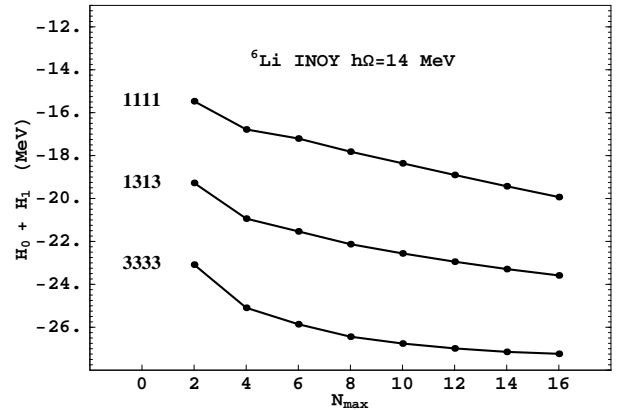


FIG. 2: The diagonal TBMEs of the sum for the core and one-body parts, $\langle ab | H_0^{6,4} + H_1^{6,5} | ab \rangle$, for the effective Hamiltonian, $\mathcal{H}_{6,6}^{0,N_{\max}}$, for ${}^6\text{Li}$ as a function of N_{\max} .

of the sum of the core and one-body parts of the effective Hamiltonian on N_{\max} starting at $N_{\max} = 6$. This means that the converged results for core plus one-body parts of the effective Hamiltonian are closely approached. The gaps in the curves are governed by the size of the spin-orbit splitting $\epsilon_1 - \epsilon_3$.

Plotting the diagonal pn TBMEs of the residual two-body part, $V_2^{6,6}$, of the effective Hamiltonian in Fig.3, we observe, that they exhibit stronger dependence than the core plus one-body parts with increase of N_{\max} . From

TABLE I: The pn TBMEs of the NCSM $H_{6,2}^{N_{\max}=12, \Omega=14}$ Hamiltonian, the p-shell effective Hamiltonians $\mathcal{H}_{6,6}^{0, N_{\max}}$ and $\mathcal{H}_{7,6}^{0, N_{\max}}$ obtained from an $N_{\max} = 12$ NCSM calculation for ${}^6\text{Li}$ are shown. The core, $H_0^{A,4}$, one-body, $H_1^{A,5}$, and residual two-body, $V_2^{A,6}$ parts for both Hamiltonians are presented. The $\mathcal{H}_{7,6}^{0, N_{\max}}$ Hamiltonian with A-independent core and one-body parts is shown in last three columns.

$2j_a$	$2j_b$	$2j_c$	$2j_d$	J	T	$H_{6,2}^{12,14}$			$\mathcal{H}_{6,6}^{0,12}$, (MeV)			$\mathcal{H}_{7,6}^{0,12}$, (MeV)			$\mathcal{H}_{7,6}^{0,12}$, (MeV)		
						A=6	A=6	A=7	$H_0^{6,4}$	$H_1^{6,5}$	$V_2^{6,6}$	$H_0^{7,4}$	$H_1^{7,5}$	$V_2^{7,6}$	$H_0^{4,4}$	$H_1^{5,5}$	$W_2^{7,6}$
1	1	1	1	0	1	-6.369	-20.528	-31.866	-54.830	36.762	-1.626	-63.336	33.614	-1.241	-30.500	11.014	-11.638
1	1	3	3	0	1	-3.818	-2.823	-3.104			-2.823			-3.104			-3.104
3	3	3	3	0	1	-9.069	-27.147	-41.661	-54.830	28.997	-0.161	-63.336	22.555	0.401	-30.500	6.535	-16.728
1	1	1	1	1	0	-7.526	-22.822	-35.152	-54.830	36.762	-3.921	-63.336	33.614	-4.526	-30.500	11.014	-14.923
1	1	1	3	1	0	-1.264	-0.645	-1.025			-0.645			-1.025			-1.025
1	1	3	3	1	0	1.724	2.012	2.107			2.012			2.107			2.107
1	3	1	3	1	0	-11.183	-27.828	-41.079	-54.830	32.879	-4.884	-63.336	28.085	-4.735	-30.500	8.774	-18.498
1	3	3	3	1	0	-4.037	-4.211	-4.977			-4.211			-4.977			-4.977
3	3	3	3	1	0	-7.180	-26.884	-41.615	-54.830	28.997	0.102	-63.336	22.555	0.448	-30.500	6.535	-16.681
1	3	1	3	1	1	-6.239	-21.419	-33.875	-54.830	32.879	1.524	-63.336	28.085	2.469	-30.500	8.774	-11.294
1	3	1	3	2	0	-10.847	-26.844	-40.884	-54.830	32.879	-3.900	-63.336	28.085	-4.540	-30.500	8.774	-18.303
1	3	1	3	2	1	-8.292	-22.951	-35.742	-54.830	32.879	-0.007	-63.336	28.085	0.602	-30.500	8.774	-13.161
1	3	3	3	2	1	1.594	1.395	1.787			1.395			1.787			1.787
3	3	3	3	2	1	-7.165	-24.892	-39.188	-54.830	28.997	2.094	-63.336	22.555	2.875	-30.500	6.535	-14.245
3	3	3	3	3	0	-9.730	-29.167	-44.520	-54.830	28.997	-2.181	-63.336	22.555	-2.457	-30.500	6.535	-19.586

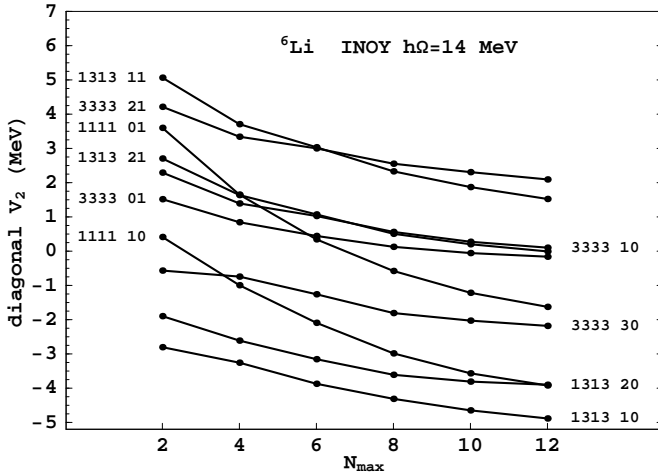


FIG. 3: The diagonal pn TBMEs of the two-body part, $\langle ab; JT | V_2^{6,6} | ab; JT \rangle$, of the effective Hamiltonian, $\mathcal{H}_{6,6}^{0, N_{\max}}$, as a function of N_{\max} .

Fig.3 we observe that the T=0 TBMEs are, on average, attractive, while the T=1 TBMEs are repulsive. Starting at $N_{\max}=6$ the two-body part shows smooth regularity. The results for nondiagonal matrix elements, shown in Fig. 4, indicates smooth, regular changes towards smaller absolute values of these TBMEs. We note that slow convergence of TBMEs with increasing N_{\max} reminds us of earlier treatment of core polarization [20, 21], where we observe slow convergence with "improved" treatments of

core-polarization within perturbation theory.

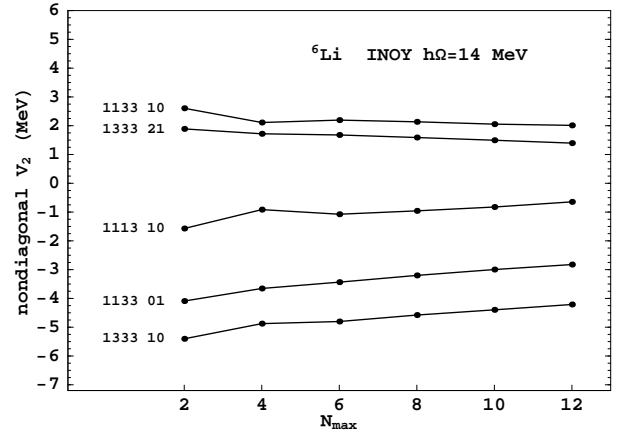


FIG. 4: The non-diagonal pn TBMEs of the two-body part, $\langle ab; JT | V_2^{6,6} | cd; JT \rangle$, for the effective Hamiltonian, $\mathcal{H}_{6,6}^{0, N_{\max}}$, as a function of N_{\max} .

A. Two-body valence cluster approximation for $A > 6$

The VCE given by the Eq.(11) would require a three-body part $V_3^{7,7}$ of the p-shell effective interaction $\mathcal{H}_{7,7}^{0, N_{\max}}$ to reproduce exactly the NCSM results for A=7 nuclei:

$$\mathcal{H}_{A=7, a_1=7}^{0, N_{\max}} = H_0^{7,4} + H_1^{7,5} + V_2^{7,6} + V_3^{7,7}. \quad (17)$$

Therefore, it is worth knowing how good the 2BVC approximation for $A=7$ as well as for $A > 7$ is. To test the 2BVC approximation, we have constructed the $\mathcal{H}_{A=7,a_1=6}^{0,N_{\max}}$ Hamiltonian, using Eq.(9), and expanded it in terms of zero-, one- and two-body valence clusters, *i.e.* omitting the three-body part:

$$\mathcal{H}_{A=7,a_1=6}^{0,N_{\max}} = H_0^{7,4} + H_1^{7,5} + V_2^{7,6}. \quad (18)$$

In other words, we have first performed NCSM calculations for the a_1 -body systems ($a_1 = 4, 5, 6$) with the $H_{A=7,2}^{N_{\max},\Omega}$ Hamiltonian. Thus, $H_0^{7,a_1=4}$ is the ${}^4\text{He}$ “core” energy and $H_1^{7,a_1=5}$ is the one-body part determined as in Eqs.(13)-(15), but with $A=7$; and $V_2^{7,a_1=6}$ is obtained by subtracting $H_0^{7,4} + H_1^{7,5}$ from $\mathcal{H}_{A=7,a_1=6}^{0,N_{\max}}$.

The resulting parts of the $\mathcal{H}_{A=7,6}^{0,N_{\max}}$ Hamiltonian are given in Table I. Comparing the TBMEs for $A=6$ and $A=7$ (Table I), we find that they differ considerably. There is a big change separately for the core and one-body parts, but weaker changes for the two-body parts, which tend to become larger in magnitude with increasing A . We have then performed SSM calculations for the ground state energy of ${}^7\text{Li}$, using the zero-, one- and two-body parts in Eq.(18). Namely, the one- and two-body parts were employed in a SSM calculation of the ground and excited states energies of the valence nucleons in the p -shell, *i.e.*, $0\hbar\Omega$ space, to which the ${}^4\text{He}$ core energy, $H_0^{7,4}$, was added, in order to yield the total energies. These calculations were repeated for $N_{\max} = 0, 2, \dots, 10$. Next we carried out NCSM calculations for ${}^7\text{Li}$ with $H_{A=7,2}^{N_{\max},\Omega}$ for the same values of N_{\max} . The SSM and NCSM results for the ground-state energy are shown in Fig.5.

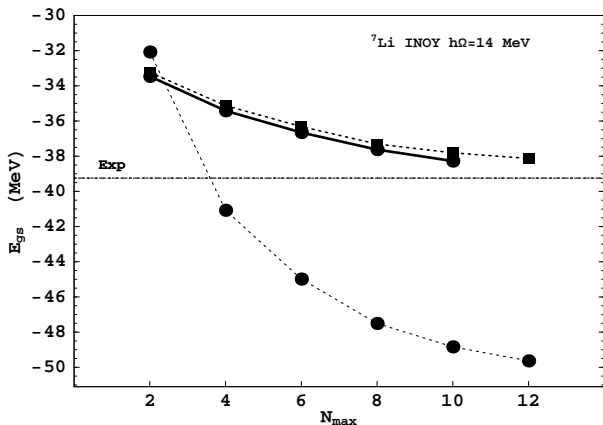


FIG. 5: The ground state energy, E_{gs} , of ${}^7\text{Li}$ as a function of N_{\max} . The NCSM results with the $H_{A=7,2}^{N_{\max},\Omega}$ Hamiltonian are shown by filled circles connected with the solid line. The SSM results with the effective $\mathcal{H}_{7,6}^{0,N_{\max}}$ Hamiltonian decomposed according to Eq.(18) are shown by squares connected with the dashed line. The SSM results with the effective $\mathcal{H}_{7,6}^{0,N_{\max}}$ Hamiltonian decomposed according to Eq.(19) are shown by filled circles connected with a dashed line.

It is also of interest to find out what would be the result if we take the fixed core and one-body parts at values which are appropriate for the $a_1 = 4$ and $a_1 = 5$ systems, respectively, because this is analogous to what is done in the SSM to determine energies relative to an inert core. To do this we adopt an alternative two-body VCE, which assumes that the core and one-body parts are A independent, *i.e.*,

$$\mathcal{H}_{A,6}^{0,N_{\max}} = H_0^{4,4} + H_1^{5,5} + W_2^{A,6}, \quad (19)$$

similar to the SSM convention given by Eq.(10). We have then performed another set of SSM calculations for $A=7$ in the same manner as described previously, but using the decomposition given in Eq.(19). To distinguish between the two-body part of the VCE given by the Eqs.(11) and (19), we have introduced the new notation, $W_2^{A,6}$, in Eq.(19). The Hamiltonian $\mathcal{H}_{7,6}^{0,12}$ expanded according to the Eq.(19) is shown in last three columns of Table I and the corresponding results are depicted in Fig.5 by the dots connected with a dashed line. Figure 5 indicates that for light systems a realistic balance of core, one-body and two-body parts of the effective interaction may be achieved only when both the core and one-body parts are mass-dependent, contrary to earlier approaches. A -independent core and one-body parts lead to a very strong two-body part for the valence nucleons and, subsequently, to drastic overbinding. It is obvious, that, in order to compensate for such an effect one would need to introduce a strongly repulsive three-body effective interaction with an unrealistic strength of about 10 MeV. Although, the effect on the spectrum is smaller, the VCE with the A -dependent core and one-body parts also yields better agreement with the exact NCSM results for the excited states. The corresponding low-energy spectrum of ${}^7\text{Li}$ obtained with the NCSM and the A -dependent SSM (using the values in columns 12,13 and 14 of Table I) are compared in Fig.6. The differences observed in

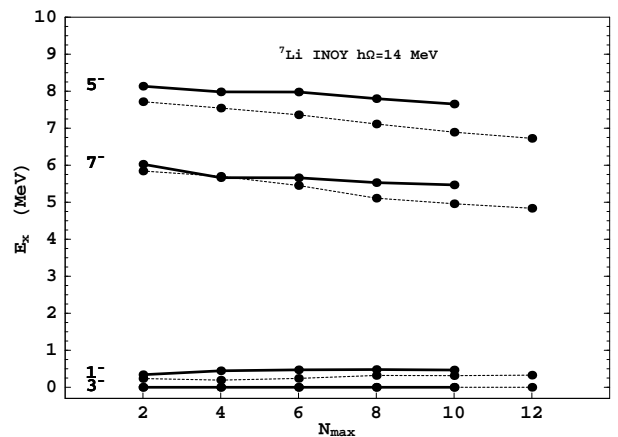


FIG. 6: NCSM (solid line) and SSM (using Eq.(18), dashed line) spectra for ${}^7\text{Li}$. The states with spin J are marked by $2J$.

Figs.5 and 6 for the ground state and excited states, re-

spectively, may be attributed to the neglected three-body part of the effective interaction at the two-body valence cluster level.

We have generalized the 2BVC expansion procedure of Eq.(18) for arbitrary mass number A ,

$$\mathcal{H}_{A,a_1=6}^{0,N_{\max}} = H_0^{A,4} + H_1^{A,5} + V_2^{A,6}, \quad (20)$$

and applied it to the $A=7,8,9$, and 10 isobars for $N_{\max}=6$. The difference of the NCSM and SSM ground state energies for different mass number A is plotted as a function of isospin projection $T_z = (N - Z)/2$ in Fig.7. Figure 7

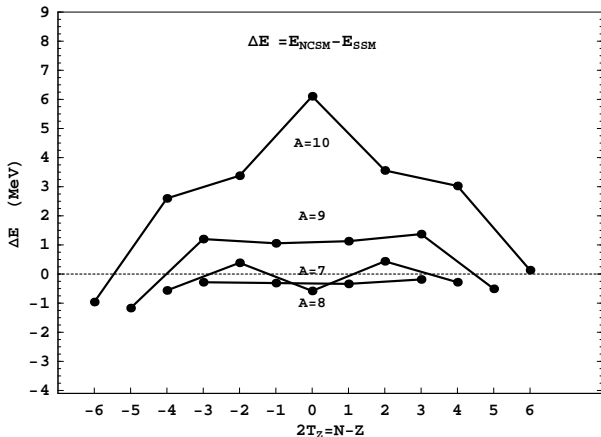


FIG. 7: The difference of the NCSM and SSM (Eq.(20)) ground state energies for different values of mass number A as a function of isospin projection $T_z = (N - Z)/2$.

shows that the three-body and higher-body correlations become more important with increasing mass number. There is also a very strong isospin dependence of the obtained results. For the highest isospin values the SSM systematically underbinds nuclei in comparison to the NCSM. However, there is an opposite effect in the vicinity of the $N = Z$ line where SSM yields considerably more binding energy than the NCSM.

Thus, the residual a_1 -body correlations with $a_1 \geq 3$ in the p-shell play an important role for $A \geq 7$ nuclei in terms of total binding energy.

B. Beyond the two-body valence cluster expansion

The analysis of the $A=7$ systems may allow us to derive an effective three-body Hamiltonian for the p-shell and to give an idea about the strength of the three-body interaction. To derive the three-body effective Hamiltonian, we employ the three-body valence cluster expansion (3BVC) approximation,

$$\mathcal{H}_{A,a_1=7}^{0,N_{\max}} = H_0^{A,4} + H_1^{A,5} + V_2^{A,6} + V_3^{A,7}, \quad (21)$$

which is the exact one for $A = 7$ systems. Comparing Eqs.(18) and (21), we find the the following result for

the three-body part $V_3^{A,7}$ of the effective Hamiltonian:

$$V_3^{A,7} = \mathcal{H}_{A,7}^{0,N_{\max}} - \mathcal{H}_{A,6}^{0,N_{\max}}. \quad (22)$$

Using Eq.(9), we derive the $A=7$ Hamiltonian, $\mathcal{H}_{7,7}^{0,N_{\max}}$, employing $a_1 = 7$ NCSM eigenvectors and eigenvalues, obtained with the $H_{7,2}^{N_{\max},\Omega}$ interaction. The same procedure is then repeated to calculate the $A=7$ Hamiltonian, $\mathcal{H}_{7,6}^{0,N_{\max}}$, employing $a_1 = 6$ NCSM eigenvectors and eigenvalues, obtained with the $H_{6,2}^{N_{\max},\Omega}$ interaction. Then, the residual three-body part $V_3^{7,7}$ is calculated according to Eq.(22). The same scheme can be applied for $A > 7$ systems taking appropriate values of A in Eq.(22).

As an example, the $T=3/2$ matrix elements of the resulting three-body effective p-shell Hamiltonian for $A=7$ and $N_{\max} = 6$ are given in Table II. On average, the nnn $T = 3/2$ Three-Body Matrix Elements (3BMEs) are attractive. They are approximately an order of magnitude smaller in absolute value than the related $T = 1$ TBMEs for $A=7$ (see Table I) and have an opposite sign. Performing the same procedure, we have obtained the 3BMEs for the $A=8, 9$ and 10 systems, which are also listed in Table II. Comparing nnn 3BMEs for different A , we note that there are only small differences; however their magnitudes become smaller for larger mass, which is in contrast to what we observed in the previous section for the two-body effective interaction.

Using obtained neutron 2BMEs and 3BMEs we have performed SSM calculations for ${}^8\text{He}$, ${}^9\text{He}$ and ${}^{10}\text{He}$, which have no valence protons and 4, 5 and 6 valence neutrons, respectively, in the p-shell. As an example, the results of the SSM calculations for ${}^8\text{He}$, ${}^9\text{He}$ and ${}^{10}\text{He}$ with effective interactions obtained in 2BVC and 3BVC approximations are compared to exact NCSM results in Table III and Fig. 8.

Obtained results indicate that the 3BVC approximation improves the agreement with the exact NCSM for the $|T_z| = 3/2, 2$ cases, i.e., for the systems where only the $T=3/2$ three-body coupling is possible. There is also considerable improvement for the excitation energies of the ${}^8\text{He}$, that is shown in Fig.8. However, to draw quantitative conclusion about the 4-body and higher-body effective interactions with $T=2, 5/2$ and 3 for identical nucleons one needs to perform exact diagonalization using 3BMEs. Figure 7 indicates also that there is a strong, and, on average repulsive 3-body effective interaction in the $T=1/2$ channel, when one has both valence protons and neutrons. We will evaluate this effect in future studies.

IV. CONCLUSION

Within the NCSM approach we can calculate, by exact projection, full A -nucleon dependent TBMEs (and 3BMEs). These A -dependent TBMEs (and 3BMEs) can be separated into core, one-body and two-body (and

TABLE II: The 3-body $T=3/2$ parts of the p-shell effective Hamiltonian, $\mathcal{H}_{7,7}^{0,N_{\max}}$, obtained from an $N_{\max} = 6$ NCSM calculation for $A=7$ isobars, ${}^7\text{He}$, ${}^7\text{Li}$, ${}^7\text{Be}$ and ${}^7\text{B}$, are shown in column 9, 10, 11 and 12, respectively. The 3-body nnn parts of the p-shell effective Hamiltonians, $\mathcal{H}_{A,7}^{0,N_{\max}}$, for $A=8, 9$ and 10 are shown in columns 13, 14 and 15, respectively. The notation $n(np)$ is used for the isospin projected combination of nnp and $nnpn$ states.

$2j_a$	$2j_b$	$2j_c$	$2j_d$	$2j_e$	$2j_f$	$2J$	$2T$	$V_{A,7}^3, (\text{MeV})$			
								$A=7$	$A=8$	$A=9$	$A=10$
								nnn	nnn	nnn	nnn
3	3	1	3	3	1	1	3	-0.055	0.181	0.354	0.471
3	3	3	3	3	3	3	3	-0.366	-0.181	-0.080	-0.026
3	3	1	3	3	1	3	3	-0.504	-0.280	-0.126	-0.030
3	1	1	3	1	1	3	3	-0.306	-0.081	-0.053	0.010
3	3	3	3	3	1	3	3	0.290	0.281	0.270	0.261
3	3	3	3	1	1	3	3	-0.246	-0.202	-0.165	-0.135
3	3	1	3	1	1	3	3	0.388	0.356	0.317	0.283
3	3	1	3	3	1	5	3	-0.209	-0.038	0.066	0.14

TABLE III: Results for ${}^8\text{He}$, ${}^9\text{He}$ and ${}^{10}\text{He}$ from SSM calculations with the effective 2BVC and 3BVC Hamiltonians and from exact NCSM calculation for $N_{\max} = 6$.

J_i^π	$E(^8\text{He}), (\text{MeV})$			J_i^π	$E(^9\text{He}), (\text{MeV})$		
	2BVC	3BVC	NCSM		2BVC	3BVC	NCSM
0_1^+	-26.323	-26.542	-26.604	$1/2_1^-$	-22.328	-22.342	-22.835
2_1^+	-21.608	-21.609	-21.752	$3/2_1^-$	-17.429	-17.452	-17.961
1_1^+	-18.555	-19.224	-19.386	0^+	$E(^{10}\text{He}), (\text{MeV})$		
0_2^+	-16.108	-16.644	-16.843		-21.219	-19.720	-21.086
2_2^+	-14.736	-15.681	-15.682				

three-body) parts, all of which are also A -dependent, contrary to the SSM approach. When these A -dependent effective one- and two-body (and three-body) interactions are employed in SSM calculations, they yield results in excellent agreement with full NCSM calculations performed in large basis spaces. Our results for $A > 7$, which include the 3-body effective interaction, indicate that 4- and higher-body effective interactions play a negligible role in determining their binding energies and spectra. Future investigations will be extended to include other physical operators, such as transition operators and EM moments.

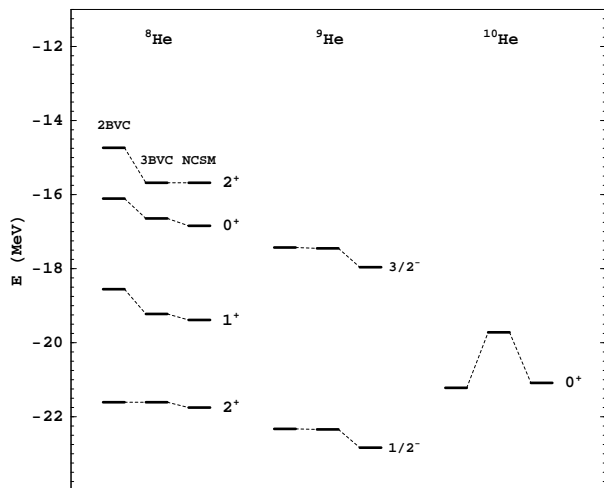


FIG. 8: Comparison of spectra for ${}^8\text{He}$, ${}^9\text{He}$ and ${}^{10}\text{He}$ from SSM calculations using the effective 2BVC and 3BVC Hamiltonians and from exact NCSM calculation for $N_{\max} = 6$.

V. ACKNOWLEDGMENTS

We thank the Institute for Nuclear Theory at the University of Washington for its hospitality and the Department of Energy for partial support during the development of this work. B.R.B. and A.F.L. acknowledge partial support of this work from NSF grants PHY0244389 and PHY0555396; P.N. acknowledges support in part by the U.S. DOE/SC/NP (Work Proposal N. SCW0498) and U.S. Department of Energy Grant DE-FG02-87ER40371; J.P.V. acknowledges support from U.S. Department of Energy Grants DE-FG02-87ER40371 and DE-FC02-07ER41457; and the work of I.S. was performed under the auspices of the U.S. DOE. Prepared by LLNL under Contract DE-AC52-07NA27344. B.R.B. thanks the Gesellschaft für Schwerionenforschung mbH Darmstadt, Germany, for its hospitality during the preparation of this manuscript and the Alexander von Humboldt Stiftung for its support.

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